

Pentanedioic acid, hexafluoro-
376-73-8 | DTXSID8059926

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 91.3 °C

Global applicability domain: Inside

Local applicability domain index: 5.91e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

Image not found

Pentanedioic acid, hexafluoro-

Measured: 80.0

Predicted: 91.3

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Hexanedioic acid, 2,2,3,3,4,4,5,5-octafluoro-

Measured: 134

Predicted: 123

Image not found

Butanedioic acid, 2,2,3,3-tetrafluoro-

Measured: 119

Predicted: 116

Image not found

1,5-Pentanediol, 2,2,3,3,4,4-hexafluoro-

Measured: 79.5

Predicted: 76.4

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3,4,5,6-Tetrafluorophthalic acid

Measured: 163

Predicted: 167